

A major purpose of the Technical Information Center is to provide the broadest dissemination possible of information contained in DOE's Research and Development Reports to business, industry, the academic community, and federal, state and local governments.

Although a small portion of this report is not reproducible, it is being made available to expedite the availability of information on the research discussed herein.

RECEIVED BY COTI MAY 06 1985
LA-UR -85-1493
CONF-850646--2

MASTER

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36

LA-UR--85-1493

TI85 010726

TITLE: CURRENT ALGORITHMS USED IN REACTOR SAFETY CODES AND THE IMPACT
OF FUTURE COMPUTER DEVELOPMENT ON THESE ALGORITHMS

AUTHOR(S): John H. Mahaffy, Applied Research Laboratory,
The Pennsylvania State University, State College, Pennsylvania 16804

Dennis R. Liles, Q-9

Susan B. Woodruff, Q-9

SUBMITTED TO: Specialists Meeting on Small Break LOCA Analyses in LWRs;
sponsored by ENEA, IAEA, NEA, and NRC;
Pisa, Italy
June 23-27, 1985

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes.

The Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. NRC.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

Los Alamos Los Alamos National Laboratory
Los Alamos, New Mexico 87545

CURRENT ALGORITHMS USED IN REACTOR SAFETY CODES AND
THE IMPACT OF FUTURE COMPUTER DEVELOPMENT ON THESE ALGORITHMS*

by

John H. Mahaffy

Applied Research Laboratory

The Pennsylvania State University

State College, Pennsylvania 16804

USA

Dennis R. Liles

and

Susan B. Woodruff

Safety Code Development

Energy Division

Los Alamos National Laboratory

Los Alamos, New Mexico 87545

USA

ABSTRACT

Computational methods and solution procedures used in the US Nuclear Regulatory Commission's reactor safety systems codes, Transient Reactor Analysis Code (TRAC) and Reactor Leak and Power Safety Excursion Code (RELAP), are reviewed. Methods used in TRAC-PF1/MOD1, including the stability-enhancing two-step (SETS) technique, which permits fast computations by allowing time steps larger than the material Courant stability limit, are described in detail, and the differences from RELAP5/MOD2 are noted.

Developments in computing, including parallel and vector processing, and their applicability to nuclear reactor safety codes are described. These developments, coupled with appropriate numerical methods, make detailed faster-than-real-time reactor safety analysis a realistic near-term possibility.

*This work was funded by the US Nuclear Regulatory Commission, Office of Nuclear Regulatory Research, Division of Accident Evaluation.

I. INTRODUCTION

In this paper we describe the computational methods used in the reactor safety codes sponsored by the US Nuclear Regulatory Commission (NRC). These methods are embedded in the Transient Reactor Analysis Code (TRAC)¹ and Reactor Leak and Power Safety Excursion Code (RELAP)² that were developed at Los Alamos National Laboratory and Idaho National Engineering Laboratory, respectively. These codes have different histories and differed significantly in their earlier versions. However, in recent years, RELAP5 has adopted a six-equation two-fluid model for two-phase flow that is quite similar to the model used in TRAC, and RELAP5/MOD2 has incorporated a variation of the stability-enhancing two-step (SETS) method^{3,4} used in the TRAC-PF1/MOD1 series for solving these equations. Because of these similarities, we describe only the TRAC-PF1/MOD1 methods in detail and note the key differences from RELAP5.

Most of the programming for these safety codes predates the availability of modern machine architectures embodying vector and parallel processing and requires changes for optimal use of current and future computers. Section IV describes trends in computer development, and Section V outlines some of the changes required for these codes to take advantage of the new machines. Fortunately, no major changes will be required in the underlying methods to use these machines effectively in the foreseeable future.

Combined use of numerical methods, such as SETS, that allow large time steps and of programming optimized for new machine architectures is an important new tool for reactor safety analysis. TRAC-PF1/MOD1 already has demonstrated the capability to analyze small-break transients of an 80-node plant model at 5 to 10 times faster than real-time using SETS in scalar mode on a Cray-1 computer. A 139-node model has been run at 1.1 times faster than real-time on a Cray X-MP with 4 central processor units (CPUs) using a version of RELAP5/MOD1 restructured for concurrent multiprocessing.⁵ By taking full advantage of stability-enhancing numerical methods and more powerful machines, both the level of detail and the calculational speed can be improved significantly. These advancements open possibilities for analysis of plant accidents while they are in progress to provide guidance to operators on the safest way to control the transient.

II. COMPUTATIONAL METHODS

The basic equations used by TRAC to model two-phase flow follow.

Liquid Mass Equation

$$\frac{\partial(1 - \alpha)\rho_\ell}{\partial t} + \nabla \cdot [(1 - \alpha)\rho_\ell \vec{V}_\ell] = -\Gamma \quad (1)$$

Combined Vapor Mass Equation

$$\frac{\partial(\alpha\rho_g)}{\partial t} + \nabla \cdot (\alpha\rho_g \vec{V}_g) = \Gamma \quad (2)$$

Noncondensable Gas Mass Equation

$$\frac{\partial(\alpha\rho_a)}{\partial t} + \nabla \cdot (\alpha\rho_a \vec{V}_g) = 0 \quad (3)$$

Solute Concentration Equation

$$\frac{\partial(1 - \alpha)m\rho_\ell}{\partial t} + \nabla \cdot [(1 - \alpha)m\rho_\ell \vec{V}_\ell] = S_c \quad (4)$$

Combined Vapor Equation of Motion

$$\begin{aligned} \frac{\partial \vec{V}_g}{\partial t} + \vec{V}_g \cdot \nabla \vec{V}_g = & - \frac{1}{\rho_g} \nabla p - \frac{c_i}{\alpha\rho_g} (\vec{V}_g - \vec{V}_\ell) |\vec{V}_g - \vec{V}_\ell| \\ & - \frac{\Gamma^+}{\alpha\rho_g} (\vec{V}_g - \vec{V}_\ell) - \frac{c_{wg}}{\alpha\rho_g} \vec{V}_g |\vec{V}_g| + \vec{g} \quad (5) \end{aligned}$$

Liquid Equation of Motion

$$\begin{aligned} \frac{\partial \vec{V}_\ell}{\partial t} + \vec{V}_\ell \cdot \nabla \vec{V}_\ell = & - \frac{1}{\rho_\ell} \nabla p + \frac{c_i}{(1 - \alpha)\rho_\ell} (\vec{V}_g - \vec{V}_\ell) |\vec{V}_g - \vec{V}_\ell| \\ & - \frac{\Gamma^-}{(1 - \alpha)\rho_\ell} (\vec{V}_g - \vec{V}_\ell) - \frac{c_{w\ell}}{(1 - \alpha)\rho_\ell} \vec{V}_\ell |\vec{V}_\ell| + \vec{g} \quad (6) \end{aligned}$$

Combined Vapor Energy Equation

$$\frac{\partial}{\partial t} (\alpha \rho_g e_g) + \nabla \cdot (\alpha \rho_g e_g \vec{V}_g) = -p \frac{\partial \alpha}{\partial t} - p \nabla \cdot (\alpha \vec{V}_g) + q_{wg} + q_{ig} + \Gamma h_{sg} \quad (7)$$

Total Energy Equation

$$\begin{aligned} \frac{\partial [(1 - \alpha) \rho_\ell e_\ell + \alpha \rho_g e_g]}{\partial t} + \nabla \cdot [(1 - \alpha) \rho_\ell e_\ell \vec{V}_\ell + \alpha \rho_g e_g \vec{V}_g] \\ = -p \nabla \cdot [(1 - \alpha) \vec{V}_\ell + \alpha \vec{V}_g] + q_{w\ell} + q_{wg} \quad (8) \end{aligned}$$

In these equations, the vapor densities and energies are sums of the steam and the noncondensable components, and we assume Dalton's law applies.

The only significant difference in the equations used in RELAP5 is the addition of virtual mass terms to the momentum equations. Our experience has been that use of appropriate virtual mass coefficients does not significantly improve calculational results, although unrealistically large coefficients can be used to damp numerical problems. Virtual mass terms have the disadvantage that each motion equation contains spatial derivatives of both liquid and vapor velocities. When applying a SETS method, these derivatives complicate the coupling between equations and result in having to solve a larger matrix for the motion equations.

To demonstrate the numerical methods used to solve these flow equations, we consider a simplified model for one-dimensional single-phase flow in a pipe. The differential equations for this model are

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho V = 0 \quad (9)$$

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot \rho e V = -p \nabla \cdot V + h (T_w - T) \quad (10)$$

and

$$\frac{\partial V}{\partial t} + V \cdot \nabla V = -\frac{1}{\rho} \nabla p - K V |V| \quad (11)$$

Here, K is a wall friction coefficient that may be a function of velocity and fluid properties, h is a heat-transfer coefficient multiplied by the heat-transfer area per volume of fluid, and T_w is a pipe wall temperature.

A staggered spatial mesh is used for the finite-difference equations with thermodynamic properties evaluated at the cell centers and the velocity evaluated at the cell edges. Only difference equations on the one-dimensional version of this mesh are demonstrated, but the generalization to two- and three-dimensional versions is not difficult. To ensure stability, flux terms at cell edges use donor-cell averages of the form,

$$\begin{aligned} \langle YV \rangle_{j+1/2} &= Y_j V_{j+1/2} \quad , \quad V_{j+1/2} \geq 0 \quad , \\ &Y_{j+1} V_{j+1/2} \quad , \quad V_{j+1/2} < 0 \quad . \end{aligned} \quad (12)$$

Here, Y may be any state variable. With this notation, the one-dimensional finite-difference divergence operator is

$$\nabla_j \cdot (YV) = \frac{(A_{j+1/2} \langle YV \rangle_{j+1/2} - A_{j-1/2} \langle YV \rangle_{j-1/2})}{\text{vol}_j} \quad , \quad (13)$$

where A is the area of the cell edge and vol_j the cell volume. The term $V \nabla V$ becomes

$$\begin{aligned} V_{j+1/2} \nabla_{j+1/2} V &= \frac{V_{j+1/2} (V_{j+1/2} - V_{j-1/2})}{\Delta x_{j+1/2}} \quad , \quad V_{j+1/2} \geq 0 \quad , \\ &\frac{V_{j+1/2} (V_{j+3/2} - V_{j+1/2})}{\Delta x_{j+1/2}} \quad , \quad V_{j+1/2} < 0 \quad , \end{aligned} \quad (14)$$

where $\Delta x_{j+1/2} = 0.5 (\Delta x_j + \Delta x_{j+1})$. This choice of $\Delta x_{j+1/2}$ for Eq. (6) is necessary for more accurate calculation of pressure drops in pipes modeled with a nonuniform mesh than is provided with a donor cell $\Delta x_{j+1/2}$.

The SETS method eliminates the material Courant stability limit by adding a stabilizer step to the basic semi-implicit solution technique. For the flow model given by Eqs. (9)-(11), the combination of basic and stabilizer equations can be written in several ways without significantly affecting the results.

When the SETS method is adapted to the two-fluid model for two-phase flow, several orderings of the difference equations can cause growing oscillations from feedback through interfacial friction terms. Some of these feedback problems are rather subtle and occur only when the one-dimensional mesh forms a closed loop. One ordering that is always stable begins with the stabilizer step for the equations of motion, continues with a solution of the basic equation set for all equations, and ends with a stabilizer step for the mass and energy equations. For this ordering, the SETS finite-difference equations for Eqs. (9)-(11) are

Stabilizer Equation of Motion

$$\begin{aligned} & \frac{(\tilde{v}_{j+1/2}^{n+1} - v_{j+1/2}^n)}{\Delta t} + v_{j+1/2}^n \nabla_{j+1/2} \tilde{v}^{n+1} + \beta (\tilde{v}_{j+1/2}^{n+1} - v_{j+1/2}^n) \nabla_{j+1/2} \tilde{v}^n \\ & + \frac{1}{\langle \rho \rangle_{j+1/2}^n \Delta x_{j+1/2}} (p_{j+1}^n - p_j^n) + K_{j+1/2}^n (2 \tilde{v}_{j+1/2}^{n+1} - v_{j+1/2}^n) |v_{j+1/2}^n| = 0 \quad , (15) \end{aligned}$$

where

$$\begin{aligned} \beta &= 0 \quad , \quad \nabla_{j+1/2} \tilde{v}^n < 0 \quad , \\ 1 & \quad , \quad \nabla_{j+1/2} \tilde{v}^n > 0 \quad ; \end{aligned}$$

Basic Equations

$$\begin{aligned} & \frac{(v_{j+1/2}^{n+1} - v_{j+1/2}^n)}{\Delta t} + v_{j+1/2}^n \nabla_{j+1/2} \tilde{v}^{n+1} \\ & + \beta (v_{j+1/2}^{n+1} - v_{j+1/2}^n) \nabla_{j+1/2} \tilde{v}^n + \frac{1}{\langle \rho \rangle_{j+1/2}^n \Delta x_{j+1/2}} (\tilde{p}_{j+1}^{n+1} - \tilde{p}_j^{n+1}) \\ & + K_{j+1/2}^n (2 v_{j+1/2}^{n+1} - v_{j+1/2}^n) |v_{j+1/2}^n| = 0 \quad ; \quad (16) \end{aligned}$$

$$\frac{(\tilde{\rho}_j^{n+1} - \rho_j^n)}{\Delta t} + \nabla_j \cdot (\rho^n \mathbf{v}^{n+1}) = 0 \quad ; \quad (17)$$

$$\begin{aligned} \frac{(\tilde{\rho}_j^{n+1} \tilde{e}_j^{n+1} - \rho_j^n e_j^n)}{\Delta t} + \nabla_j \cdot (\rho^n e^n \mathbf{v}^{n+1}) \\ + \tilde{p}_j^{n+1} \nabla_j \cdot (\mathbf{v}^{n+1}) - \bar{h}_j^n (T_{wj}^n - \tilde{T}_j^{n+1}) = 0 \quad ; \end{aligned} \quad (18)$$

and

Stabilizer Mass and Energy Equations

$$\frac{(\rho_j^{n+1} - \rho_j^n)}{\Delta t} + \nabla_j \cdot (\rho^{n+1} \mathbf{v}^{n+1}) = 0 \quad ; \quad (19)$$

$$\begin{aligned} \frac{(\rho_j^{n+1} e_j^{n+1} - \rho_j^n e_j^n)}{\Delta t} + \nabla_j \cdot (\rho^{n+1} e^{n+1} \mathbf{v}^{n+1}) \\ + \tilde{p}_j^{n+1} \nabla_j \cdot (\mathbf{v}^{n+1}) - \bar{h}_j^n (T_{wj}^n - \tilde{T}_j^{n+1}) = 0 \quad . \end{aligned} \quad (20)$$

A tilde above a variable indicates that it is the result of an intermediate step and is not the final value for the time step. The material Courant stability limit is eliminated by treatment of the terms $\mathbf{V}\mathbf{V}\mathbf{V}$, $\nabla \cdot \rho \mathbf{V}$, and $\nabla \cdot \rho e \mathbf{V}$ during the two steps. Additional robustness has been obtained with the particular form for the friction terms and the use of nonzero values of β in the $\mathbf{V}\mathbf{V}\mathbf{V}$ terms. These special terms for friction and $\mathbf{V}\mathbf{V}\mathbf{V}$ are obtained by linearizing similar terms that are fully implicit in velocity ($K_{j+1/2}^n \mathbf{v}_{j+1/2}^{n+1} |\mathbf{v}_{j+1/2}^{n+1}|$ and $\mathbf{v}_{j+1/2}^{n+1} \nabla_{j+1/2} \mathbf{v}_{j+1/2}^{n+1}$).

Equations (16-18) are very similar to a one-dimensional single-phase version of the difference equations traditionally used for the TRAC vessel component. These semi-implicit equations can be obtained by dropping all tildes from Eqs. (16)-(19) and replacing the $\mathbf{V}\mathbf{V}\mathbf{V}$ and friction terms in Eq. (16) with $\mathbf{v}_{j+1/2}^n \nabla_{j+1/2} \mathbf{v}_{j+1/2}^n$ and $K_{j+1/2}^n \mathbf{v}_{j+1/2}^n |\mathbf{v}_{j+1/2}^n|$, respectively. The differences between the one- and three-dimensional equations have been eliminated in the nuclear plant analyzer (NPA)⁶ extension of TRAC. With this most recent extension of the

code, the three-dimensional difference equations are a straightforward generalization of the original one-dimensional SETS equations.

The RELAPS equations differ from this version because they eliminate Eq. (15) and evaluate the spatial difference of velocity in Eq. (19) at the new time level. This change provides the most efficient way of dealing with the presence of the virtual mass terms in the full two-fluid equations.

The heat-transfer term $\bar{h}^n(T_w^n - T^{n+1})$ is written in this form to minimize coupling between the hydrodynamic and heat-transfer solution procedures. To maintain stability in regions of rapid change in h , \bar{h}^n is an average of the heat-transfer coefficient evaluated at time level n and the averaged coefficient from level $n-1$ ($\bar{h}^n = 0.45 h^n + 0.55 \bar{h}^{n-1}$). An experimental version of TRAC-PF1/MOD1 exists with fully implicit heat-transfer terms [$\bar{h}^{n+1}(T_w^{n+1} - T^{n+1})$]. Current versions of RELAPS evaluate T_w at the new time level.

Equation (15) simply represents a tridiagonal linear system in the unknown \bar{v}^{n+1} and is solved first. Next, the coupled nonlinear system given by Eqs. (16)-(18) is solved. An important difference between TRAC and RELAP is that TRAC proceeds with an iterative solution of these nonlinear equations whereas RELAP solves only the first linear approximation. Details of the solution procedure for these equations are presented in Sec. III. Once these equations are solved, \bar{v}^{n+1} is known; hence, Eqs. (19) and (20) are simple tridiagonal linear systems, with unknowns ρ_i^{n+1} and ρ_{i+1}^{n+1} , respectively. When this equation set is adapted to flow in complex piping networks or to multidimensional flow, the tridiagonal structure is lost. However, the matrices are still sparse and easily solved.

A standard linear stability analysis predicts unconditional stability for this set of difference equations; this result has been verified by a large number of computational test problems. However, at very large time steps, functional forms for the friction factor containing a strong velocity dependence can drive instabilities, as can a strong void-fraction dependence for interfacial friction in the two-fluid model. This is why the method is referred to as stability enhancing rather than unconditionally stable.

Because the basic form of the finite-difference operators (both spatial and temporal) is consistent between the two steps, the order of accuracy of the full SETS equations is the same (first order in space and time) as the basic semi-implicit Eqs. (16)-(18). This consistency appears necessary to prevent feedback oscillations between the two steps. It also has the advantage of ensuring that, for modest time-step sizes, the results of any SETS calculation approach those of the basic semi-implicit equations.

The SETS method is especially valuable when applied to the full two-fluid model for two-phase flow. For this model, the stabilizer equations add less than 20% to the computational cost per cell per step of the basic equation set. A fully implicit method multiplies this cost by a factor of 6. The full finite-difference equations for the two-fluid model are given in the TRAC-PF1/MOD1 manual.

III. SOLUTION OF THE BASIC EQUATION SET

For TRAC, the first step in the solution of the basic (semi-implicit) equation set rearranges the motion equation to obtain the new time velocity as a linear function of new time pressures. For Eq. (16), this step results in the relation,

$$v_i^{n+1} = \frac{v_i^n - \Delta t [v_i^n \nabla_i (\tilde{v}^{n+1} - \beta \tilde{v}^n) - K_i^n v_i^n |v_i^n| + \frac{\tilde{p}_{j+1}^{n+1} - \tilde{p}_j^{n+1}}{\langle \rho \rangle_i^n \Delta x_i}]}{1 + \Delta t (2K_i^n |v_i^n| + \beta \nabla_i \tilde{v}^n)} \quad (21)$$

where $i = j + 1/2$. Given this relation, the derivatives of velocity with respect to pressure are

$$\frac{dv_{j+1/2}^{n+1}}{dp_j^{n+1}} = \frac{\Delta t}{\langle \rho \rangle_i^n \Delta x_i (1 + K_i^n \Delta t |v_i^n| + \Delta t \beta \nabla_i \tilde{v}^n)} \quad (22)$$

and

$$\frac{dv_{j+1/2}^{n+1}}{dp_{j+1}^{n+1}} = - \frac{dv_{j+1/2}^{n+1}}{dp_j^{n+1}} \quad (23)$$

Equation (21) and thermodynamic equations giving $\rho(p,T)$ and $e(p,T)$ are substituted into Eqs. (17) and (18) to give a coupled system of nonlinear equations with unknowns p_j^{n+1} and T_j^{n+1} (tildes have been dropped to simplify notation). Solution of this system is obtained with a standard Newton iteration. Given the latest estimates of p_j^{n+1} and T_j^{n+1} for pressures and temperatures, we assume the solution is

$$p_j^{n+1} = p_j'^{n+1} + \delta p_j \quad (24)$$

and

$$T_j^{n+1} = T_j^{n+1} + \delta T_j \quad (25)$$

After substituting Eqs. (21)-(25) into the basic equation set, making the necessary Taylor series expansions, and discarding nonlinear terms in δp_j and δT_j , the resulting linear mass and energy equations are

$$\begin{aligned} \frac{\partial \rho'}{\partial T} \Big|_j^{n+1} \delta T_j + \frac{\partial \rho'}{\partial p} \Big|_j^{n+1} \delta p_j - \left(\frac{A_{j+1/2} \rho_{j+1/2}^n \Delta t}{V_{01j}} \frac{dV_{j+1/2}^{n+1}}{dp_j^{n+1}} \right) (\delta p_{j+1} - \delta p_j) \\ - \left(\frac{A_{j-1/2} \rho_{j-1/2}^n \Delta t}{V_{01j}} \frac{dV_{j-1/2}^{n+1}}{dp_j^{n+1}} \right) (\delta p_j - \delta p_{j-1}) \\ = \rho_j^n - \rho_j^{n+1} - \Delta t \nabla_j \cdot (\rho^n \mathbf{V}^{n+1}) \quad ; \end{aligned} \quad (26)$$

and

$$\begin{aligned} (\rho_j^{n+1} \frac{\partial e'}{\partial T} \Big|_j^{n+1} + e_j^{n+1} \frac{\partial \rho'}{\partial T} \Big|_j^{n+1} + \Delta t \bar{h}_j^{n+1}) \delta T_j \\ + (\rho_j^{n+1} \frac{\partial e'}{\partial p} \Big|_j^{n+1} + e_j^{n+1} \frac{\partial \rho'}{\partial p} \Big|_j^{n+1} + \Delta t \nabla_j \cdot \mathbf{V}^{n+1}) \delta p_j \\ - (p_j^{n+1} + \rho_{j+1/2}^n e_{j+1/2}^n) \left(\frac{A_{j+1/2} \Delta t}{V_{01j}} \frac{dV_{j+1/2}^{n+1}}{dp_j^{n+1}} \right) (\delta p_{j+1} - \delta p_j) \\ - (p_j^{n+1} + \rho_{j-1/2}^n e_{j-1/2}^n) \left(\frac{A_{j-1/2} \Delta t}{V_{01j}} \frac{dV_{j-1/2}^{n+1}}{dp_j^{n+1}} \right) (\delta p_j - \delta p_{j-1}) \\ = \rho_j^n e_j^n - \rho_j^{n+1} e_j^{n+1} \\ - \Delta t [\nabla_j \cdot \rho^n e^n \mathbf{V}^{n+1} + p_j^{n+1} \nabla_j \cdot \mathbf{V}^{n+1} - \bar{h}_j^n (T_{w,j}^n - T_j^{n+1})] \quad . \end{aligned} \quad (27)$$

The normal procedure for starting this linearization is to make an initial estimate for the new time pressure and temperature of $p^{n+1} = p^n$ and $T^{n+1} = T^n$. However, when SETS is used, an extra call to the thermodynamic subroutines can be saved by taking $p^{n+1} = p^n$ and $T^{n+1} = T^n$.

Equations (26) and (27) can be abbreviated as

$$B_j \begin{pmatrix} \delta p_j \\ \delta T_j \end{pmatrix} = \underline{b}_j + \underline{c}_j(\delta p_{j+1} - \delta p_j) - \underline{d}_j(\delta p_j - \delta p_{j-1}) \quad (28)$$

where B is a 2×1 matrix. For the one-dimensional numerics, this equation is multiplied by B^{-1} in the first step of the solution (accomplished with a linear system solver), which yields

$$-d'_{1,j} \delta p_{j-1} + (1 + d'_{1,j} + c'_{1,j}) \delta p_j - c'_{1,j} \delta p_{j+1} = b'_{1,j} \quad (29)$$

and

$$\delta T_j = b'_{2,j} + c'_{2,j}(\delta p_{j+1} - \delta p_j) - d'_{2,j}(\delta p_j - \delta p_{j-1}) \quad (30)$$

where $\underline{b}' = B^{-1}\underline{b}$, etc. All coefficients are stored, and then the set of equations represented by Eq. (29) is solved for all δp_j . Finally, the known values for pressure variations are substituted into Eq. (30) to obtain temperature changes and used with Eqs. (22) and (23) to obtain updated velocities. Given these changes, the next estimates for new time pressures and temperatures are generated and used to obtain densities and energies. If changes in δT and δp are too large, these estimates are used in Eqs. (24) and (25) to relinearize for another iteration of the one-dimensional equations. As previously noted, the three-dimensional flow equations are not relinearized. In this case, time-step controls are used to assure the accuracy of a single linearization.

Note from the form of Eqs. (26) and (27) that the Jacobian for the system is reevaluated on each iteration. This reevaluation may not always be necessary but, for steam-water flows with phase change, it is often important for rapid convergence of the iteration.

The RELAPS solution procedure is necessarily different. The basic mass and energy equations are solved to obtain the fundamental variables as functions of the unknown new time cell-edge velocities. This solution provides a linear relation between the pressure and velocities, which is substituted into the finite-difference momentum equation to obtain a linear system with only velocities as the unknowns. When two-fluid equations are solved, this procedure results in a single linear system coupling both liquid and vapor velocities with twice the bandwidth of the standard SETS matrices.

IV. COMPUTER HARDWARE

Until recently, the dominant computer architecture has been the simple serial computer. On this machine, each instruction of a given type must be complete before the next instruction of this type can be initiated. For example, if two different additions must be performed, the first pair of numbers is provided to the adder; then, the computer must wait until the result is stored before the second pair of numbers can be sent to the adder.

One improvement over standard serial processing has been available for about 25 years. With the pipelining process, it is possible to send a second pair of numbers to the adder before the result of the first addition is available. Consequently, the total time for the two additions can be significantly less than twice the time required to complete a single addition. This advantage improves with multiplication, but the original pipelined machines did not provide this feature for division.

The main disadvantage of the original pipelining concept was that no systematic method was provided to keep the pipelines full. This problem has been addressed with modern vector processors such as the Cray-1, CYBER 205, FACOM VP-100, and Hitachi S810/20. Hardware and compiler features that recognize when long strings of operations are available for pipeline processing have been provided. A vector processor carries out identical computations on a set of array elements. Consequently, a disadvantage of these vector machines is that a substantial amount of care must be devoted to coding of algorithms and, in some cases, to choosing the type of algorithm to take full advantage of the vector features. Software for automatic conversion of existing codes to take advantage of vector processing is still quite primitive. Such conversion produces source code that appears quite different from the original and is difficult to modify and debug. Also, automatic converters cannot take advantage of information that is not in the code but may be readily available to the programmer. However, sophisticated interactive vectorizers, such as that developed by Fujitsu⁶ in Japan, are rapidly decreasing the programmer time required to vectorize existing code as well as to develop new vectorized code. These new vectorizers allow the programmer to incorporate global information relevant to vectorization in the form of compiler directives and provide clear explanations of the reasons for failure to vectorize.

Serial, and to some extent vector, computers have remained the dominant machines for high-speed computing for 40 years largely because of the rapid improvement in the speed of the electronic circuitry. In recent years, the rate of improvement in basic processor speed has slowed dramatically, and some see hardware reaching basic speed limits.⁹ These limitations have accelerated the use of parallel processing as a means to achieve very high net computational speeds. The basic idea behind parallel processing is that, if there are several independent operations to perform, they can be done concurrently on separate processors. A parallel processor differs from a vector processor in that the parallel or concurrent computations do not have to be identical. All major supercomputer manufacturers are working toward machines with 4 to 16 vector processors, and some are now offering the 4-processor units. Research continues on machines with far more units, some having a thousand or more units. Again, these new architectures require new software, and development of appropriate software tools for parallel computing is an active area of current research.

The advent of new machine architectures opens the way for faster-than-real-time detailed analysis for possible accident mitigation and recovery. A less obvious advantage of parallel processing lies in calculations for applications such as licensing. Both TRAC and RELAP are used on Control Data Corporation (CDC) 7600 computers to provide important information to the US NRC that can be used to make licensing decisions. With the generation of 32-bit processor chips and 64-bit floating-point coprocessors that are currently moving into production, it will be possible to construct a small and inexpensive parallel machine (four to eight units) with at least the speed of a CDC 7600. This new hardware will expand the availability of TRAC and RELAP as analysis tools. As the combination of hardware and software improves, an important basis for improved nuclear plant simulators will be provided.

V. IMPACT OF NEW HARDWARE ON SAFETY CODES

Both TRAC and RELAP were written primarily for serial computation. The major exception is the coding for the new three-dimensional SETS vessel in TRAC-NPA, which was written with vectorization in mind. Optimal adaptation of these codes to vector and parallel machines will be time-consuming. However, projects are underway to improve the performance of both codes on the new-generation computers. Fortunately, the underlying equations and methods in these codes lend themselves well to both vector and parallel processing. Calculation of all heat-transfer and friction coefficients are independent as are the setup and initial reduction of the flow equations. The only complication occurs in the solution of the TRAC pressure equation system [Eqs. (17) and (18)] or the analogous RELAP5 velocity system (versions of RELAP5 without SETS also have pressure equations). However, methods exist for efficient solution of these equations on vector and parallel machines, and TRAC currently employs a partitioning technique for the solution of the system in one-dimensional components that adapts easily to parallel processing.

RELAP5/MOD1 has been vectorized for efficient use of a FACOM VP-100 and runs from 2.4 to 2.8 times faster than the original scalar version.⁶ The reprogrammed portion involved 10,000 lines and accounted for 91% of the computing time in the original scalar calculation. A similar estimate has been made for the amount of reprogramming necessary to attain a comparable speedup for TRAC-PF1/MOD1 on Cray computers.

The reprogramming effort is less if only parallel processing is required. Approximately 1,000 lines need to be changed or added to use 2 to 16 parallel processors effectively. A subset of TRAC, which models flow in a single pipe, has been the subject of extensive testing in the heterogeneous-element-processor (HEP) architecture and was 93% parallelized by self-scheduling cell computations.⁶ This same subset showed a 3.5 speedup on a four-processor Cray X-MP/48 using some experimental microtasking constructs. A project to parallelize the full TRAC NPA version is in progress. Numerical experiments performed on a Cray X-MP/48 using the full RELAP5/MOD1 version already have shown wallclock performance improvements of 1.5 to 3.0 resulting from multiprocessing.⁶

Although most near-term changes to TRAC and RELAP will be devoted to increasing the speed of existing models, very high computational speed also will permit a level of detail in modeling not previously possible. For example, the

addition of more difference equations to allow detailed time-dependent modeling of flow regimes, front-tracking of concentration gradients, detailed models of the growth of thermal boundary layers at vertically stratified interfaces, and a model of turbulent mixing would be desirable.

VI. CONCLUSIONS

The use of improved numerical methods in the NRC's reactor safety system codes, combined with code optimization for new supercomputer architectures, will allow best-estimate engineering simulation at substantially faster than real-time. When combined with new microprocessor technology, these codes will be available to a wider range of engineers for detailed plant analysis, often running close to real-time. Thus, new opportunities for safety analysis, operator training, and accident mitigation will be created.

REFERENCES

1. "TRAC-PF1/MOD1: An Advanced Best-Estimate Computer Program for Pressurized Water Reactor Thermal-Hydraulic Analysis," Los Alamos National Laboratory report LA-10157-MS, NUREG/CR-3858 (to be published).
2. V. H. Ransom, et al., "RELAP5/MOD2 Code Manual, Vol. I: Code Structure, Systems Models, and Solution Methods," Idaho National Engineering Laboratory report EGG-SAAM-6377 (April 1984).
3. J. H. Mahaffy, "A Stability-Enhancing Two-Step Method for Fluid Flow Calculation," J. Comput. Phys. 46, 329 (1982).
4. J. A. Trapp, R. A. Riemke, and R. J. Wagner, "Nearly-Implicit Hydrodynamic Numerical Scheme and Partially Implicit Hydrodynamic and Heat Slab Coupling for RELAP5/MOD2," Idaho National Engineering Laboratory report EGG-CMD-6715 (1984).
5. H. Makowitz, "Numerical Experiments in Concurrent Multi-processing with the RELAP5 Nuclear Reactor Systems Code," Eleventh International Meeting on Advances in Nuclear Engineering Computational Methods, Knoxville, Tennessee (1985).
6. R. G. Steinke, C. P. Booker, P. T. Giguere, D. R. Liles, J. H. Mahaffy, M. R. Turner, and R. A. Wiley, "The Nuclear Plant Analyzer: An Interactive TRAC/RELAP Power-Plant Simulation Program," Los Alamos National Laboratory report LA-UR-84-2953 (1984).
7. F. A. Addessio, "Improved Coupling of the Conduction and Flow Equations in TRAC," Transactions of the ANS, 39, 494 (1981).
8. M. I. Shiguro, H. Harada, N. Shinozawa, and K. Naraoka, "Vectorization of LWR Transient Analysis Code RELAP5/MOD1 and Its Effect," Japan Atomic Energy Research Institute report JAERI-M 85-040 (1985).
9. O. M. Lubeck, P. O. Frederickson, R. E. Hiromoto, and J. W. Moore, "The Los Alamos Experiences with the HEP Computer," Los Alamos National Laboratory report LA-UR-84-3442 (1984).